

NIST Releases a Thermodynamic and Transport Properties Database for Ionic Liquids: ILTHERMO

NIST announced the public release of ILThermo (NIST Standard Reference Database 147) in July 2006. ILThermo is a free web research tool that allows users worldwide to access an up-to-date data collection from the publications on experimental studies of thermodynamic and transport properties of ionic liquids, as well as binary and ternary mixtures containing ionic liquids. The inaugural version contains information on more than 200 ions and 300 ionic liquids.

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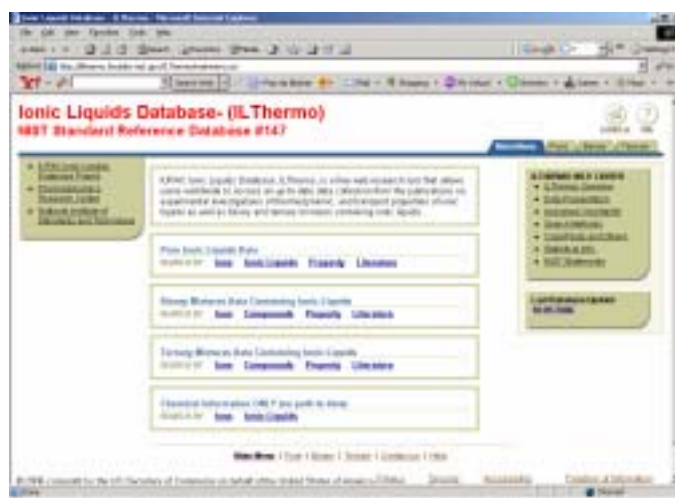
There has been an explosion of interest in the last few years (including a near-exponential growth in journal articles) in the synthesis and use of ionic liquids – salts that melt below the boiling point of water. With typical vapor pressures in the range of 10^{-10} Pa, ionic liquids have essentially no vapor emissions, and so look like excellent candidates for “green solvents” to replace hazardous, air-polluting organic solvents such as acetone and benzene. With dozens of anions and cations to choose from, they can be tailored to specific needs and may be particularly useful as solvents for biocatalysis. Progress in utilizing ionic liquids has been hampered by the lack of an open-access, public-domain, comprehensive data retrieval system scoped to cover information pertaining to ionic liquids. Development of such a database infrastructure encompasses a number of complex issues related to data submission, processing, mining, quality control, management, critical evaluation, and dissemination. In 2003, an International Union of Pure and Applied Chemistry established its Task Group to conduct the project 2003-020-2-100 “Ionic Liquids Database” with an objective to “create an open-access, free, on-line, comprehensive database for storage and retrieval of metadata and numerical data for ionic liquids, including their syntheses, structure, properties, and uses; lack of this information is impeding progress in a burgeoning field of significant current interest”.

In July 2006, ILThermo (NIST Standard Reference Database 147) was released to the public as a result of the development initiated at NIST in close cooperation with the

IUPAC. ILThermo is a free web research tool that allows users worldwide to access an up-to-date data collection from the publications on experimental studies of thermodynamic and transport properties of ionic liquids, as well as binary and ternary mixtures containing ionic liquids.

The inaugural version of ILTHERMO contains information on more than 200 ions and 300 ionic liquids. The collected data cover the relevant literature from 1982 to 2006 for pure ionic liquids as well as for binary and ternary systems containing ionic liquids. The database contains more than 18000 experimental data points.

The experimental data stored in the database include those for phase transitions, transport, volumetric, and thermal properties as well as electrical conductivity, surface tension, refractive index, speed of sound, vapor pressure, and activity coefficients. The database presently contains more than 18000 experimental data points. The information available from ILThermo includes chemical identification, numerical property values, details of experimental methods, sample purity, and uncertainty. The database is made available to the public with the use of a Web-Oracle data dissemination system recently established at NIST. In order to increase efficiency and enforce strict data quality control for the data collection process of the thermophysical properties of ionic liquids, the NIST TRC Group modified its Guided Data Capture software to incorporate the elements of metadata specifically important for ionic liquids. The data generated by ILThermo can easily be downloaded from the Web and propagated into a variety of the chemical engineering software applications.



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